



Thermoelectric properties of SbNCa_3 and BiNCa_3 for thermoelectric devices and alternative energy applications

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ABSTRACT

Thermoelectric properties of two antiperovskites SbNCa_3 and BiNCa_3 are calculated using first principles calculations. High values of Seebeck coefficients are observed for these materials. Electrical and thermal conductivities are also calculated. Increase in thermal conductivity and decrease in electrical conductivity are found with increasing temperature. The maximum values of thermal conductivity are $92 \times 10^{14} \text{ W/m K s}$ and $88 \times 10^{14} \text{ W/m K s}$ for SbNCa_3 and BiNCa_3 respectively at a temperature of 900 K. The peak values of $5 \times 10^{20} / \Omega \text{ m s}$ and $5.2 \times 10^{20} / \Omega \text{ m s}$ are achieved for n-type SbNCa_3 and BiNCa_3 respectively at a temperature of 300 K. Figure of merit is achieved for these materials at room temperature which shows that these materials can be useful for thermoelectric devices and alternative energy sources.

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1. Introduction

Energy crisis around the world has forced researchers to find alternative sources of energies and energy saving materials and devices. The field of thermoelectric (TE) materials has gained importance in the last decade for its ability to solve energy crisis all around the globe. TE compounds are considered as the compounds that can solve the problems of power generation and refrigeration technologies [1–4]. These compounds are also useful in smart sensors, energy harvesting, and the new concept of thermo-power wave sources [5–9]. In thermoelectric power generators, thermal energy is directly converted into electrical energy [10] and thus acts as good sources of green energy. High quality and good TE materials are used and required for power generation and other thermoelectric applications depend upon the nature

of the materials [11,12]. Good TE materials have large electrical conductivity and Seebeck coefficient, while they have small thermal conductivity. Figure of merit, $ZT = \sigma S^2 T / k$, represents the condition for better TE materials; where S is the Seebeck coefficient, σ is the electrical conductivity and k is the thermal conductivity [13,14] and power factor, $P = S^2 \sigma$ represents the electrical properties of the materials [15].

Different materials with diverse crystal structures possess thermoelectric properties. Skutterudites [16], Clathrates [17], Half-Heusler Alloys [18], Chalcogenides [19] and Complex Oxide structured materials have been reported by numerous researchers [20, 21]. Perovskites are also reported to be suitable TE materials and potential candidates in this field [22,23]. Weidenkaff et al. [24] experimentally studied the effects on thermoelectric properties of Ca doping in LaCoO_3 perovskite. Wilfried et al. [25] investigated TE properties of NaTaO_3 based perovskites. For Nb doped SrTiO_3 the confined electron gas has been successfully investigated and it is proved that their Seebeck coefficients are ten times larger than bulk materials [26–28]. Flahaut et al. [29] worked on structure and thermoelectric properties of polycrystalline samples $\text{Ca}_{1-x}\text{A}_x\text{MnO}_3$ ($A = \text{Yb, Tb, Nd and Ho}$). However, the TE properties of antiperovskite materials, which have perovskite type structure, have not been investigated yet. A wide variety of semiconductors show good

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thermoelectric properties [30–32] and there are many antiperovskites materials which are semiconductors in nature.

In the present work, we have investigated the TE properties of two antiperovskite materials SbNCa_3 and BiNCa_3 at 300, 600 and at 900 K temperatures. Chern et al. [33] reported experimentally that these two compounds are semiconductors having lattice constants of 4.8541 Å and 4.888 Å for SbNCa_3 and BiNCa_3 , respectively. In our previous theoretical work [34] we have verified their structural and electronic results and showed a band gap of approximately 1.1 eV for these materials. Our studies also show that there are dense electronic states at Fermi level in valance band and in conduction band especially. Due to the small band gap and dense electronic states at Fermi level, we consider these materials to be good candidates for TE applications. Thermoelectric results, investigated in this report, show that our predictions are correct. All thermoelectric properties like Seebeck coefficients, electrical conductivity, thermal conductivity and figure of merit prove that these materials are excellent candidates for TE applications. However, there are no experimental or theoretical results to be compared with but we hope that this paper will open new avenues of studies for the researchers.

2. Computational details

We investigated the electronic properties of SbNCa_3 and BiNCa_3 using the FP-LAPW method within the sphere of the density functional theory (DFT) [35,36] as implemented in the WIEN2k package [37]. The details of the FP-LAPW method and cubic perovskite unit cell for each compound are provided in our previous work [34]. The separation energy between core and valance states was set at -6.0 Ry. l_{max} , Rk_{max} and G_{max} are set equal to 10, 7 (RMT) $^{-1}$ and 14 (a.u.) $^{-1}$ respectively. k points equal to 2300 were used in irreducible Brillouin zone. Electronic properties were calculated by LDA, GGA, EVGGA and mBJ. We showed that mBJ exchange potential [38,39] gives the best results for band gap so in this manuscript, for calculating thermoelectric properties, we used electronic properties calculated by mBJ. In the present work, thermoelectric properties like Seebeck coefficients, thermal conductivities and electrical conductivities are calculated using BoltzTrap [40] code. Eq. (1) interprets transport coefficients, which are based on the rigid band approach to conductivity:

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{1}{N} \sum_{i,k} \sigma_{\alpha\beta}(i, k) \frac{\delta(\varepsilon - \varepsilon_{i,k})}{\delta(\varepsilon)} \quad (1)$$

$$\sigma_{\alpha\beta}(i, \vec{k}) = e^2 \tau_{i,k} v_{\alpha}(i, \vec{k}) v_{\beta}(i, \vec{k}) \quad (2)$$

where, N is the number of k -points. Eq. (2) explains K -dependent transport tensors where τ is the relaxation time, and $v_{\alpha}(i, \vec{k})$ is a component of group velocities. As a function of temperature, T , and chemical potential, μ , the transport coefficients like the electrical conductivity and Seebeck coefficient tensors can be found by integrating the transport distribution [40,41]:

$$\sigma_{\alpha\beta}(T, \mu) = \frac{1}{\Omega} \int \sigma_{\alpha\beta}(\varepsilon) \left[-\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (3)$$

$$S_{\alpha\beta}(T, \mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T, \mu)} \int \sigma_{\alpha\beta}(\varepsilon)(\varepsilon - \mu) \times \left[-\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (4)$$

where, α and β are the tensor indices, e is the electron charge, Ω is volume of the unit cell, μ is carrier concentration and f_0 is Fermi–Dirac distribution function. τ , the relaxation time, is one of the basic input for the calculation of thermoelectric properties and

in this study we take it as a constant. Seebeck coefficient does not depend on relaxation time thus can be calculated by band structure calculation but electrical conductivity needs to be calculated with respect to the relaxation time.

3. Results and discussion

3.1. Seebeck coefficient

Potential difference is created in Seebeck effect between two different conductors or semiconductors in successive contact when there is a temperature gradient between the two junctions. Potential difference is developed because of the movements of free electrons from the higher temperature region towards the lower temperature region. This electronic movement causes thermoelectromotive force which produces voltage in micro volts per Kelvin. The developed voltage depends on the nature of the materials and the movement of electrons in the material. Figure of merit depends on the Seebeck coefficient so for a good thermoelectric device we need a large Seebeck coefficient.

Fig. 1(a) and (b) represent curves of Seebeck coefficients for SbNCa_3 and BiNCa_3 respectively at 300 K, 600 K and 900 K. We can see that the highest value of Seebeck coefficient for both the materials is achieved at room temperature. Both materials exhibit approximately same behavior. For p-type SbNCa_3 and BiNCa_3 , Seebeck coefficients have the maximum values of 1740 $\mu\text{V/K}$ and 1730 $\mu\text{V/K}$ respectively at 300 K, which shows that these are good thermoelectric materials. It is clear from the figure that Seebeck coefficient decreases almost exponentially with temperature. Similar behavior is observed for n-type SbNCa_3 and BiNCa_3 , which shows that these materials are as good in n-type as in p-type. The peaks are obtained between -0.5 and 0.5 $\mu(\text{eV})$ chemical potential, while beyond these points Seebeck coefficient drops rapidly to zero which means these materials will exhibit good thermoelectric properties between these points.

3.2. Thermal conductivity

Electrons and lattice vibrations are responsible for the conduction of heat in a material. In semiconductors, heat is transferred mostly because of lattice vibrations while in metals free electrons are good source of thermal conductivity [42]. For a good thermoelectric device, thermal conductivity should be small so that temperature gradient could be maintained. Fig. 2(a) and (b) present thermal conductivities for SbNCa_3 and BiNCa_3 respectively at 300 K, 600 K and 900 K as a function of chemical potential. Same behavior is observed for both materials. It is clear from the figures that thermal conductivity for room temperature remains approximately zero between -0.4 and 0.4 $\mu(\text{eV})$ chemical potential for both materials. This is the region where these materials can give maximum efficiency. Thermal conductivity increases when one move away from $\mu = 0$. Explanation for this may be given from the basic definition of chemical potential μ . When one atom is placed in an element and you want to place another, the first one will oppose the second. Similarly when a third atom is placed the first two will oppose. This opposition of the already placed atoms in an element or compound to the new incoming atoms is called chemical potential. When chemical potential increases then repulsion to the incoming atoms also increases, causing more lattice vibration. This increased lattice vibration results in high conductivity. Similarly if chemical potential is negative that means a new entering atom is welcomed by the already present atoms in the element or compound and hence attraction occurs. Because of the attraction again lattice vibration increases as there is a force involved. This causes an increase in thermal conductivity. When chemical potential is negligibly small then repulsive or attractive force is also

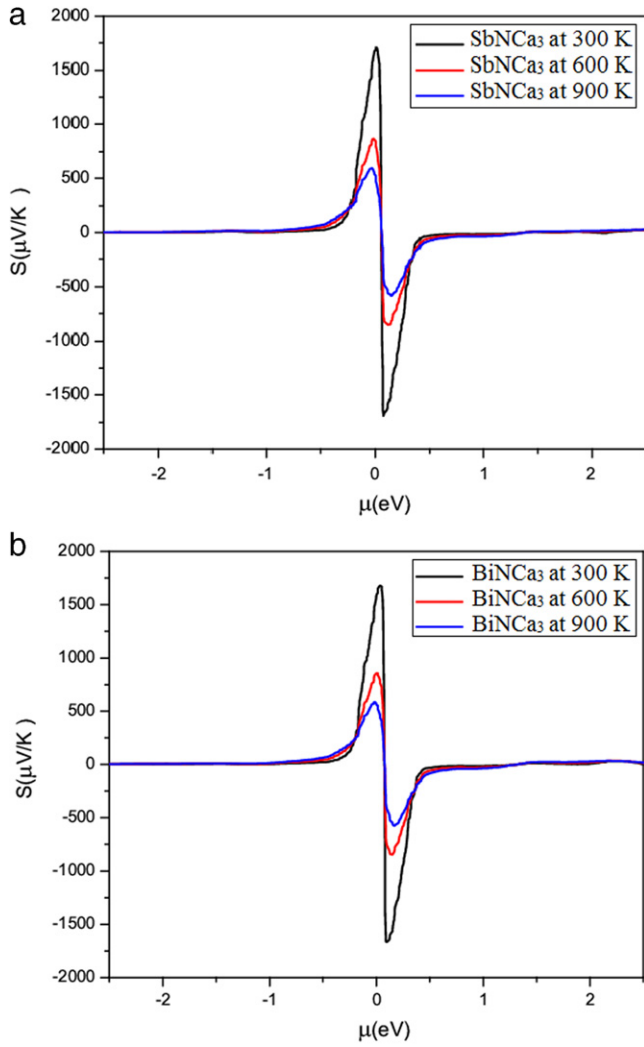


Fig. 1. Seebeck coefficients for (a) SbNCa_3 and (b) BiNCa_3 at 300, 600 and 900 K.

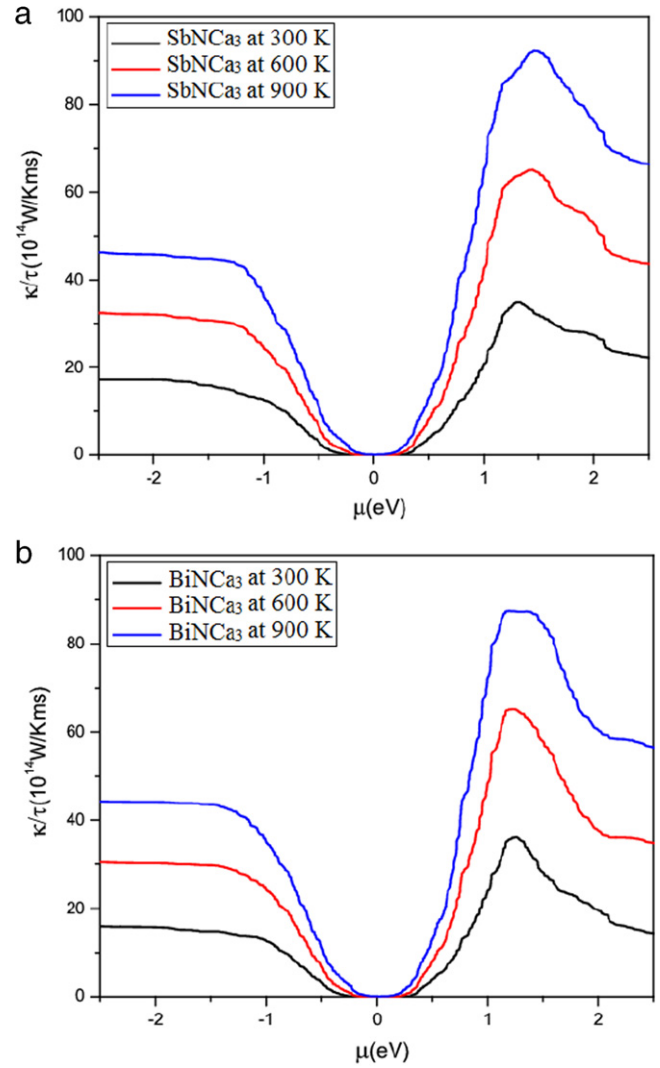


Fig. 2. Thermal conductivities for (a) SbNCa_3 and (b) BiNCa_3 as a function of chemical potential.

small resulting less vibrations and hence small conductivity. Further, we see that thermal conductivity has lower values in p-type materials as compared to n-type. At 300 K the peak values are $18 \times 10^{14} \text{ W/K m s}$ and $16 \times 10^{14} \text{ W/K m s}$ for p-type SbNCa_3 and BiNCa_3 respectively.

3.3. Electrical conductivity

Electrical conductivity can be attributed as the measure of flow of free charge carriers in a material. Free electrons, on gaining heat, gain kinetic energy and move towards the colder part of the material thus producing electric current. For a good thermoelectric device, materials should have high electrical conductivity to reduce Joule heating effect [16]. Fig. 3(a) and (b) represent electrical conductivities for SbNCa_3 and BiNCa_3 respectively at 300, 600 and 900 K. Both materials show approximately same behavior at given temperatures. It is clear from the figure that $-0.3 \mu(\text{eV})$ and $0.3 \mu(\text{eV})$ chemical potentials are the critical points for electrical conductivity in p-type and n-type materials respectively. It means that material will give good thermoelectric properties beyond these points. The figure shows that leaving a small range of chemical potential in the vicinity of $\mu = 0$, both materials have good electrical conductivities for all other values of chemical potential. The peak values

of $5 \times 10^{20}/\Omega \text{ m s}$ and $5.2 \times 10^{20}/\Omega \text{ m s}$ are achieved for n-type SbNCa_3 and BiNCa_3 respectively at $1.3 \mu(\text{eV})$ chemical potential.

3.4. Figure of merit

The performance of a thermoelectric material can be predicted by its figure of merit (ZT), which is directly proportional to high Seebeck coefficient and electrical conductivity, while inversely proportional to the thermal conductivity. Mathematically, figure of merit is given by,

$$ZT = \sigma S^2 T / \kappa \quad (5)$$

S is the Seebeck coefficient, σ is the electrical conductivity and κ is thermal conductivity

Materials having ZT about unity or greater than unity are considered excellent candidates for thermoelectric devices [42,43]. Fig. 4(a) and (b) shows the graph for ZT and chemical potential for SbNCa_3 and BiNCa_3 respectively. ZT shows approximately same behavior for both materials. It is clear from the figure that at room temperature ZT is very close to unity, which shows these materials can be used for thermoelectric applications. ZT sharply rises as chemical potential increases from zero, and the peak value is observed at -0.1 and $0.1 \mu(\text{eV})$ chemical potentials for both materials. This is because Seebeck coefficient gives maximum

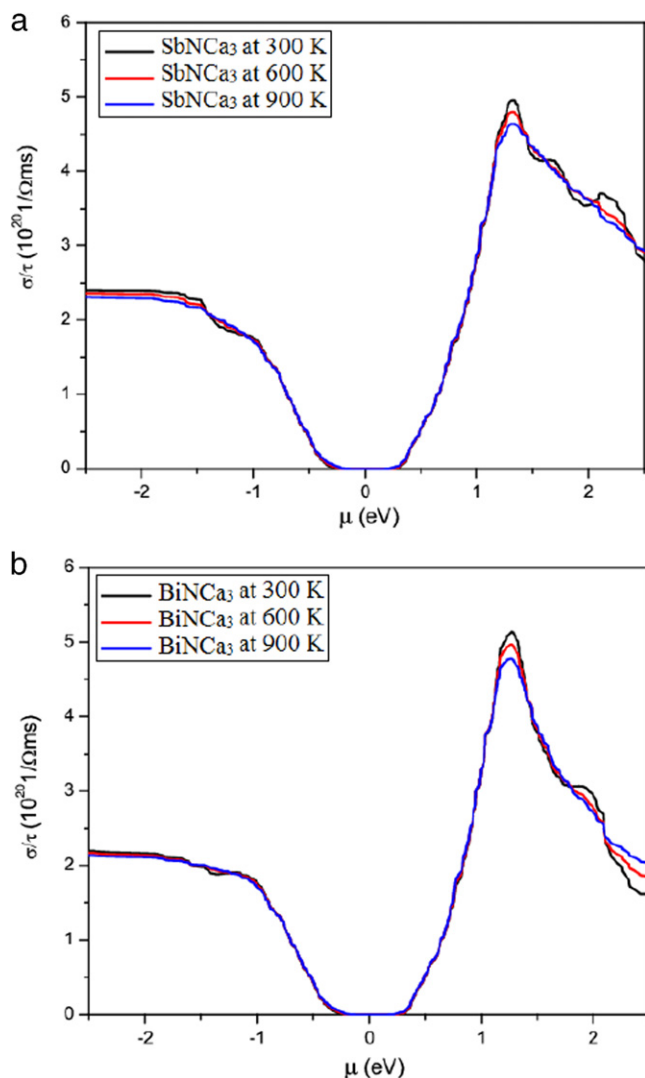


Fig. 3. Electrical conductivities for (a) SbNCa_3 and (b) BiNCa_3 as a function of chemical potential at 300, 600 and 900 K.

values and thermal conductivity stays at minimum at -0.1 and $0.1 \mu(\text{eV})$ chemical potentials. Beyond these points ZT decreases and drops to 0.2 at -0.4 and $0.4 \mu(\text{eV})$ chemical potentials. The reason for this may be the sharp increase in thermal conductivity beyond these points. In p-type region of these materials, ZT becomes zero beyond $-1 \mu(\text{eV})$ chemical potential but in n-type we see small values between 1.2 and 2.5 $\mu(\text{eV})$ chemical potential. The reason for this difference is the fact that the electrical conductivity reaches to maximum values between these points.

4. Conclusion

Thermoelectric properties of SbNCa_3 and BiNCa_3 are calculated for the first time in this study. We have obtained very interesting results for these materials at room temperature. Very high Seebeck coefficients are obtained between -0.5 and 0.5 chemical potential while thermal conductivities are zero in this region. So, we find peak values for figure of merit in this region. Electrical conductivity gives maximum value between 1.2 and 2.5 chemical potential. For this reason, we see small values of figure of merit in this region. The overall pattern of figure of merit clearly shows these are good thermoelectric materials and can be used for electricity production and as alternative energy sources.

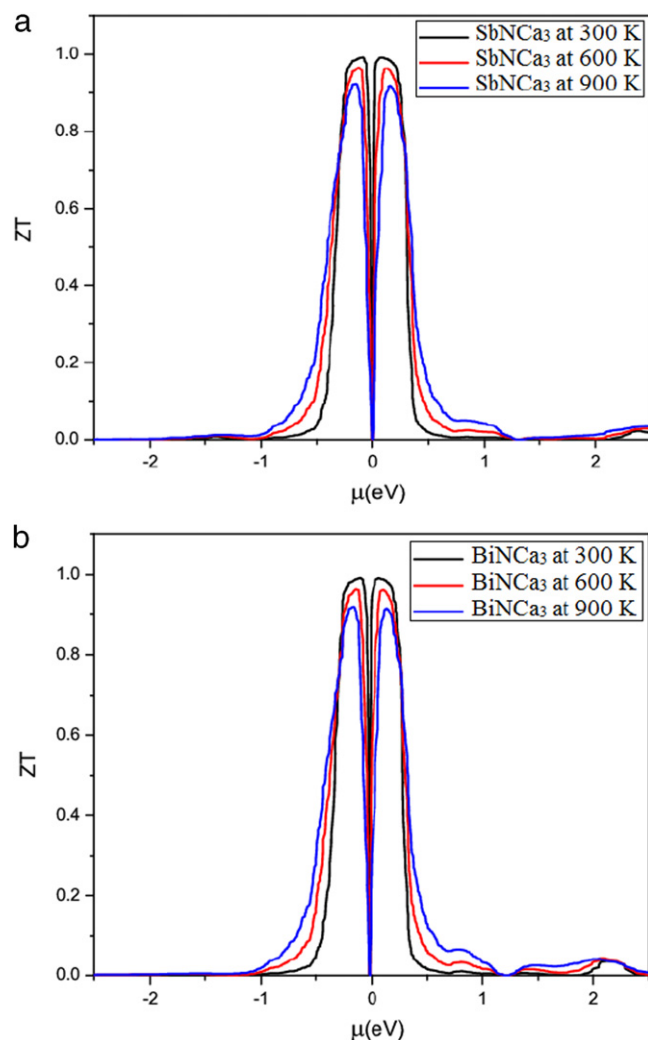


Fig. 4. Graph for ZT vs chemical potential for (a) SbNCa_3 and (b) BiNCa_3 .

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